

## Chemical effects of diffusive mixing in protoplanetary disks

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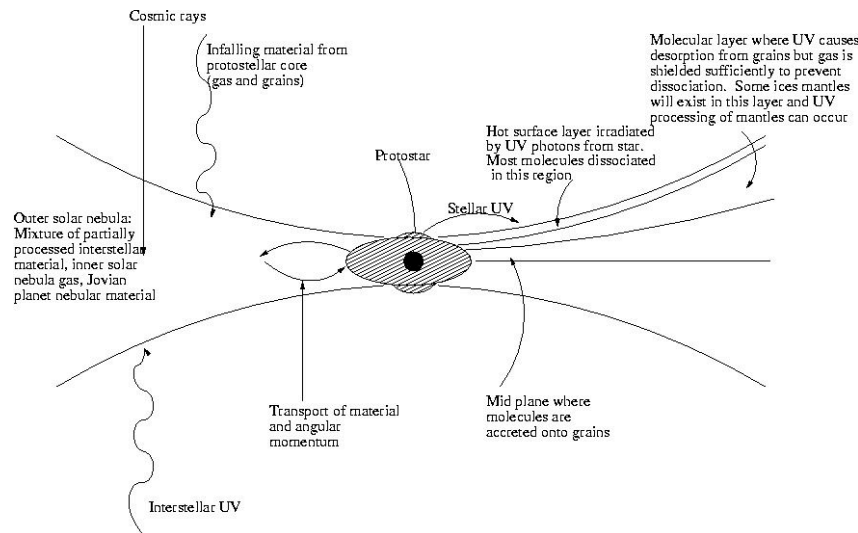
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### Summary

We report preliminary results from models of protoplanetary disks that consider the effects of diffusive mixing on the chemistry. We find that mixing in the vertical direction can have a considerable effect on the predicted column densities for reasonable values of the diffusion coefficient,  $D$ , estimated from the viscosity coefficient,  $\alpha$ . The abundances of most species are increased with the addition of diffusion, but a few, including HCN are decreased at some radii. The calculated column densities for models with only thermal desorption are considerably lower than those observed, indicating that mixing alone cannot account for the observations and that more efficient desorption processes, e.g. photodesorption must be included in the models.

### Introduction

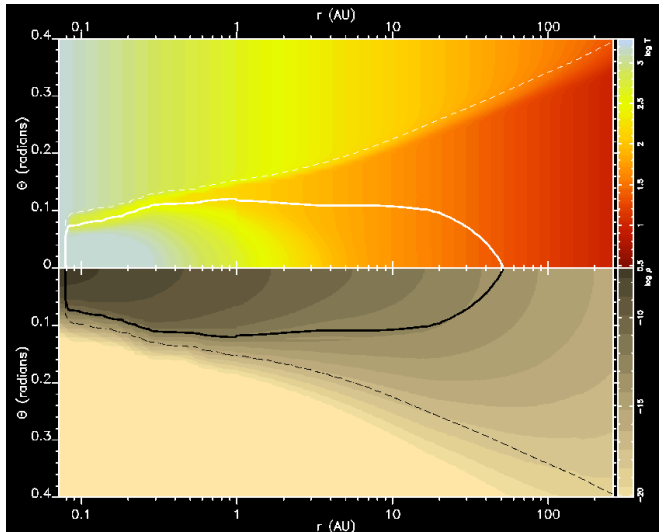
Models of the chemistry of protoplanetary disks show that the disk can be divided vertically into three distinct layers (Willacy & Langer 2001, Aikawa et al. 2002) (Figure 1). Mixing within the disk could allow transport of material between the layers.



**Figure 1:** The chemical structure of an irradiated, flared, protoplanetary disk, showing how it is divided vertically into three chemically distinct layers. At the surface, the strong UV field removes mantles from the grains and dissociates gaseous molecules into their constituent atoms and ions. Below this is a layer where molecules are sufficiently shielded from the UV to prevent them from being dissociated. Finally in the mid-plane the high density and low temperature ensure that most molecules are frozen onto dust grains.

## The model

### Hydrodynamical model: Bryden et al. (2004)

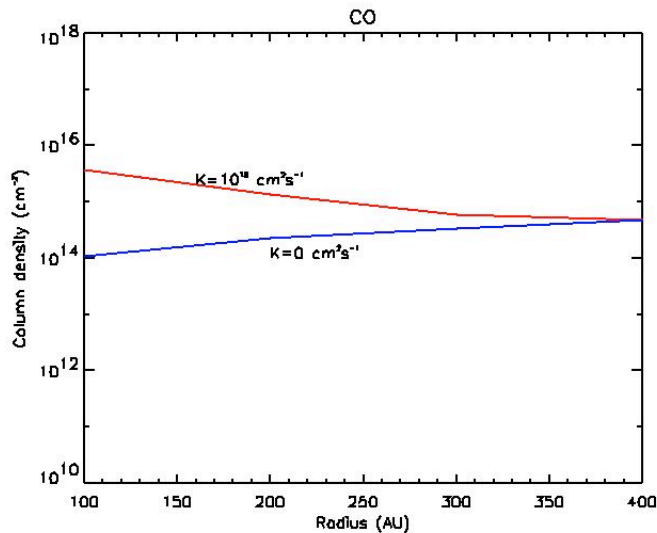


**Figure 1:** The disk structure as calculated by Bryden et al. (2004) for a model with mass accretion rate =  $10^{-8} M_{\odot}$  and  $\Sigma_0 = 1000 \text{ g cm}^{-2}$  at 1 AU. The model calculates the temperature self-consistently and includes surface irradiation and viscous dissipation towards the mid-plane. The top panel shows temperature in the disk and the bottom panel the density structure. The solid dark line shows the surface of the disk based on the vertical depth of its own infrared radiation, while the dotted line plots the optical surface to radial, visible stellar radiation.

- **Diffusion model** - 1-D turbulent mixing code previously used to model molecular clouds by Willacy et al. (2002) and Xie et al. (1995)
- **Chemical model** - subset of UMIST database RATE95 (Millar et al. 1997). Input abundances from a molecular cloud model run to 1 Myrs (most molecules are accreted onto grains at start of disk model).
- **Diffusion coefficient** - estimated by  $K = \alpha c_s h$  (Morfill 1983, Stevenson 1990) where  $\alpha$  is the parameter used to describe the viscosity in the hydrodynamical model,  $c_s$  is the sound speed and  $h$  is the disk scale height.  $K$  assumed to be constant with  $R$  and  $z$  in our models,

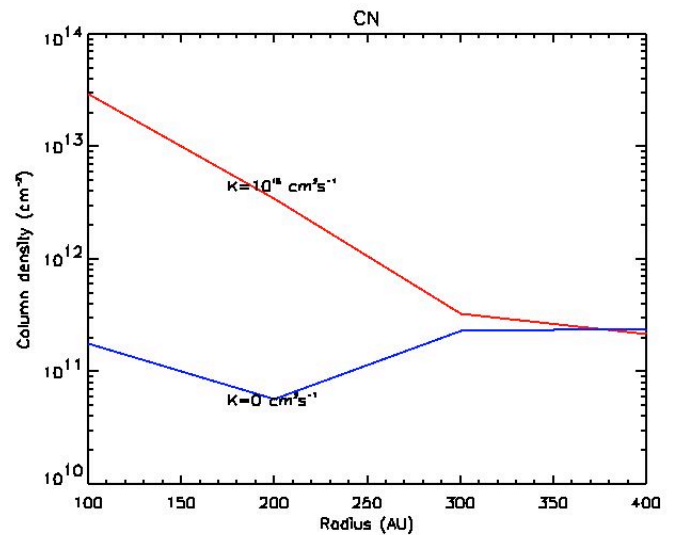
## Results

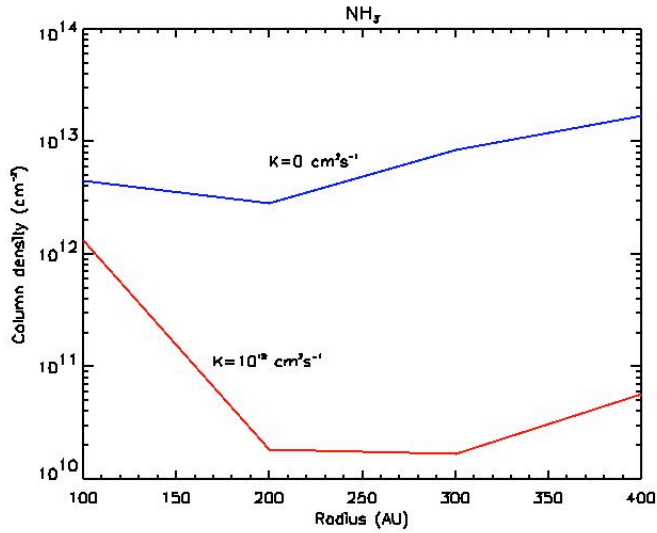
- Diffusion increases the depth of the molecular layer (Figure 1).
- Most molecules show an increase in column density when diffusion is included.
- Nitrogen-bearing molecules especially  $\text{NH}_3$  are an exception



- Low column density of CO due to either the choice of input abundances (molecules frozen on grains) or the lack of efficient, non-thermal desorption.
- With diffusion, movement of grains into the warm surface layer causes desorption of volatile species e.g. CO,  $\text{CH}_4$ . Dissociation of  $\text{CH}_4$  leads to production of radicals such as CH which react with O to form CO. Hence diffusion increases CO abundance and  $N(\text{CO})$  increases as R decreases (and temperature/desorption increase).

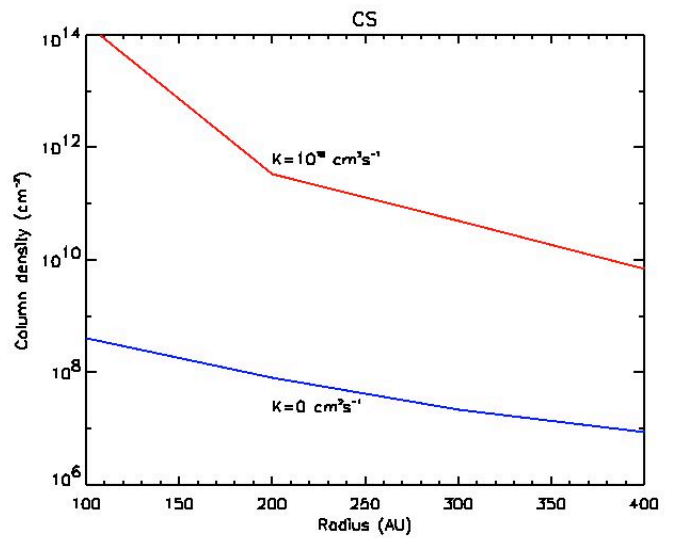
- CN also shows an increase in column density at  $R < 400$  AU for diffusion model
- Increase in diffusion model due to evaporation of grain mantles as they are transported towards the surface, releasing HNC which is processed into CN by UV photodissociation and by reaction with  $\text{C}^+$ .





- Large decrease in  $N(\text{NH}_3)$  in outer disk.
- Diffusion increases the  $\text{H}_3^+$  abundance, which increases the destruction rate of  $\text{N}_2$  in the disk and increases the formation of  $\text{NH}_3$ .  $\text{NH}_3$  is less volatile than  $\text{N}_2$  and remains on the grains once frozen out. In  $K=0$  model, the more volatile  $\text{N}_2$  provides a source of nitrogen throughout the disk

- Diffusion causes an increase in  $N(\text{CS})$ , which extends to larger radii than other molecules.



These results show the importance of including diffusion processes in calculating vertical chemical profiles in disks

## **References**

- Aikawa et al. (2002) A&A **386** 622  
Bryden, G., Lin, D., Yorke, H. & Velusamy, T. (2004) (in preparation)  
Millar, T., Farquhar, P. & Willacy, K. (1997) A&AS **121** 139  
Morfill, G. E. (1983) Icarus **53** 41  
Stevenson, D. (1990) ApJ **348** 730  
Willacy, K. & Langer, W. (2001) ApJ, **544** 903  
Willacy, K., Langer, W. & Allen, M. (2002) ApJ **573** L119  
Xie, T., Allen, M. & Langer, W. (1995) ApJ **440** 674

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